35th Annual Students' Symposium

12-13 April 2022

ABSTRACT BOOKLET

Department of Materials Engineering

Indian Institute of Science, Bangalore - 560012

Organising Committee

Faculty Co-ordinator:

Prof. Chandan Srivastava

Convenors:

Swapnil S Bhure

Akhand Pratap Singh

Mohan Guttula

Volunteers:

Apoorva Singh

Anooj Sathyan

Ashutosh Panchal

Sudeepta Mukherjee

Faizan Hijaji

Sashidhar G

Yash Bajpai

Maadhav

Symposium Schedule (at a glance)

Day 1: Tuesday, 12 April 2022	
9:45 - 10:00	Welcome address
10:00-10:45 (Invited Talk 1)	Prof. Vikram Gavini
10:45-11:00	High Tea
11:00-13:00 Platform presentation (Session 1)	
11:00-11:20	Sushma Indrakumar
11:20-11:40	Dereje Bekele Tekliye
11:40-12:00	Saswat Choudhury
12:00-12:20	Suryakanta Mondal
12:20-12:40	Reshma Devi
12:40-13:00	Pritiranjan Mondal
13:00-14:00	Lunch Break
14:00-16:00 Platform presentation (Session 2)	
14:00-14:20	Faizan Hijazi
14:20-14:40	Suhela Isaac Tyeb
14:40-15:00	Tirthesh Ravindra Ingale
15:00-15:20	Sazid Khan
15:20-15:40	Ferdin Sagai Den Bosco
15:40-16:00	Jinu Joji
16:00-16:15	High Tea
16:15-17:00 (Invited Talk 2)	Prof. Vijay Chandru

Day 2: Wednesday, 13 April 2022	
10:00-10:45 (Invited Talk 3)	Prof. Pavan Nakula
10:45-11:00	High Tea
11:00-13:20 Platform presentation (Session 3)	
11:00-11:20	Aashranth Bommakanti
11:20-11:40	Saurabh Kumar Gupta
11:40-12:00	Deepak Kumar
12:00-12:20	Hemant Kumar
12:20-13:00	Akshat Godha
12:40-13:00	Deepak Deelip Patil
13:00-13:20	Sushma Kumari
14:30-15:45 Poster Presentation	
15:45-16:00	High Tea
16:00-16:45 (Invited Talk 4)	Prof. Vilupanur A. Ravi
16:45-17:00	Valediction
19:00 onwards	Dinner at the Department

Detailed Symposium Schedule

DAY 1: Tuesday, 12 April 2022	
9:45 - 10:00	**Welcome Address**
Invited Talk-1 (10:00-10:45)	
10:00-10:45	**Towards Large-scale Quantum Accuracy Materials Simulations** Vikram Gavini *Department of Mechanical Engineering, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, USA*
High Tea (10:45-11:00)	
Platform Presentation Session 1 (11:00-13:00)	
11:00-11:20	**Rapid Blood Clotting with Silica/Silk Fibroin-Composite Based Bilayered Foam** Sushma Indrakumar[a], Santanu Ghosh[a], Tapan Dash[b], Vivek Mishra[b], Bharat Tandon[b] Kaushik Chatterjee[a] *[a] Department of Materials Engineering, Indian Institute of Science, Bangalore, India* *[b] Fibroheal Woundcare Pvt. Ltd., Bangalore, India*
11:20-11:40	**Exploration of NaSICON frameworks as calcium-ion battery cathodes** Dereje Bekele Tekliye and Sai Gautam Gopalakrishnan *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
11:40-12:00	**4D Printing of Multifunctional Biocompatible Magnetic Composites** Saswat Choudhary, Kaushik Chatterjee *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
12:00-12:20	**Investigation of thin-film delafossite materials for energy efficient memory devices** Suryakanta Mondal, Dr. Bhagwati Prasad *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
12:20-12:40	**Effect of Exchange-Correlation Functionals on the Estimation of Migration Barriers in Battery Materials** Reshma Devi, Baltej Singh, Pieremanuele Canepa, and Gopalakrishnan Sai Gautam *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
12:40-13:00	**Injectable and Self-Healing Polysaccharide-based Hydrogels for Sustained and Localized Delivery** Pritiranjan Mondal and Kaushik Chatterjee *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
Lunch Break (13:00-14:00)	

Platform Presentation Session 2 (12:00-16:00)	
14:00-14:20	**Micro-Texture Regions in Rolled Ti-6Al-4V Under Polarized Light** Faizan Hijazi[a], Dheepa Srinivasan[b], Barna Roy[a], Praveen Kumar[a] and Vikram Jayaram[a] [a] *Department of Materials Engineering, Indian Institute of Science, Bangalore, India* [b]Pratt & Whitney, Research and Development Center, Bangalore – 560012 (India)
14:20-14:40	**Gelatin-Sericin-Laminin Cryogels for Tissue Regeneration in Diabetic Wounds** Suhela. T,[a] Parvaiz A. Shiekh,[a]1 V. Verma[d,e], and A. Kumar.[a,c] [a]*Department of Biological Science and Bioengineering, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India.* [b]*Centre for Environmental Sciences and Engineering,* [c]*Centre for Nanosciences,Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India* [d] *Centre for Environmental Sciences and Engineering,* [e] *Materials Science and Engineering,Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India.*
14:40-15:00	**Plasticity development and crack nucleation analysis under dwell fatigue loading of Ti 6242 by using ECCI** Tirthesh Ingale, Dipankar Banerjee *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
15:00-15:20	**Ballistic impact failure characteristics of Al 2024-T351** Sazid Khan, S. Karthikeyan *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
15:20-15:40	**An investigation of multiphase flows through a packed bed with implications to iron-making blast furnaces** Ferdin Sagai Don Bosco, Govind S. Gupta *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
15:40-16:00	**Design of a polymer encapsulating film to prevent lead leakage from lead perovskite solar cells** Jinu Joji, Praveen C Ramamurthy *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
High Tea (16:00-16:15)	
Invited Talk-2 (16:15-17:00)	
16:15-17:00	**Innovation in Indian Science: Lessons from Covid-19** Vijay Chandru *Centre for BioSystems Science and Engineering, Indian Institute of Science, Bangalore, India*

DAY 2: Wednesday, 13 April 2022	
Invited Talk-3 (10:00-10:45)	
10:00-10:45	**Insights into unconventional ferroelectricity in hafnia-based systems through operando STEM and XRD** Pavan Nakula *Center for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India*
High Tea (10:45-11:00)	
Platform Presentation Session 3 (11:00-13:00)	
11:00-11:20	**A phase transformation in steel during hot deformation: unique features revealed through crystallographic texture** B. Aashranth [a,b] , Dipti Samantaray[b] , Satyam Suwas[a] [a] *Department of Materials Engineering, Indian Institute of Science, Bangalore, India* [b] *Metallurgy and Materials Group, Indira Gandhi Centre for Atomic Research, Kalpakkam*
11:20-11:40	**Directed energy deposition of a low modulus TNZT alloy for biomedical applications** Saurabh Kumar Gupta[a], Kaushik Chatterjee[a], Satyam Suwas[a] [a]*Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
11:40-12:00	**Role of characterisation techniques in understanding the microstructure of metal additive manufacturing** Deepak Kumar[a], Soumita Mondal[a], KG Prashanth[b,c,d], Satyam Suwas[a] [a] *Department of Materials Engineering, Indian Institute of Science, Bangalore, India* [b]*Department of Mechanical and Industrial Engineering, Tallinn University of Technology, Ehitajate Tee5, 19086, Tallinn, Estonia* [c]*Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria* [d]*CBCMT, School of Mechanical Engineering, Vellore Institute of Technology, Tamil Nadu, India*
12:00-12:20	**Understanding creep deformation behavior of extruded Mg-Ce alloys** Hemant Kumar, Surendra Kumar Makineni *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
12:20-12:40	**Controlled electron channeling contrast imaging of defects in engineering alloys** Akshat Godha, Surendra Kumar Makineni *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
12:40-13:00	**Engineered nanotopography on 3D-printed polymer scaffolds to impart mechanobactericidal property** Deepak Patil, Kaushik Chatterjee *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
13:00-13:20	**3D Bioprinting of Photo-crosslinkable Kappa-Carrageenan to Fabricate Cell-loaded Tissue Scaffolds** Sushma Kumari, P. Mondal, and K. Chatterjee *Department of Materials Engineering, Indian Institute of Science, Bangalore, India*

Lunch Break (13:20-14:30)	
Poster Presentation (14:30-15:45)	
High Tea (15:45-16:00)	
Invited Talk-4 (16:00-16:45)	
16:00-16:45	**Natural Materials - A Tale of Two Explorations** Vilupanur A. Ravi *Department of Chemical and Materials Engineering, California State Polytechnic University, Pomona (Cal Poly Pomona), USA*
16:45-17:00	**Valediction**
Dinner at the Department from 19:00 onwards	

Invited Speakers

Towards Large-scale Quantum Accuracy Materials Simulations

Vikram Gavini

Professor, Department of Mechanical Engineering, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, USA

Abstract:

Electronic structure calculations, especially those using density functional theory (DFT), have been very useful in understanding and predicting a wide range of materials properties. The importance of DFT calculations to engineering and physical sciences is evident from the fact that ~20% of computational resources on some of the world's largest public supercomputers are devoted to DFT calculations. Despite the wide adoption of DFT, and the tremendous progress in theory and numerical methods over the decades, the following challenges remain. Firstly, the state-of-the-art implementations of DFT suffer from cell-size and geometry limitations, with the widely used codes in solid state physics being limited to periodic geometries and typical simulation domains containing a few hundred atoms. This limits the complexity of materials systems that can be treated using DFT calculations. Secondly, there are many materials systems (such as strongly-correlated systems) for which the widely used model exchange-correlation functionals in DFT, which account for the many-body quantum mechanical interactions between electrons, are not satisfactory. Addressing these challenges will enable large-scale quantum-accuracy DFT calculations, and can significantly advance our ab initio modeling capabilities to treat complex materials systems.

This talk will discuss our recent advances towards addressing the aforementioned challenges. In particular, the development of computational methods and numerical algorithms for conducting fast and accurate large-scale DFT calculations using adaptive finite-element discretization will be presented, which form the basis for the open-source DFT-FE code. The computational efficiency, scalability and performance of DFT-FE will be presented, which demonstrates a significant outperformance of widely used plane-wave DFT codes. Some recent studies that highlight the capabilities of DFT-FE will be presented, which include: (i) studies on dislocation energetics in Magnesium; (ii) understanding the electronic structure underpinnings of electron transport in DNA molecules. In addressing the second challenge, our recent breakthrough in accurately solving the inverse DFT problem will be presented, which has enabled the computation of exact exchange-correlation potentials for polyatomic systems. Ongoing efforts on using the exact exchange-correlation potentials to develop a data-driven approach for improving the exchange-correlation functional description in DFT will be discussed.

This is joint work with Sambit Das (U. Michigan), Bikash Kanungo (U. Michigan) and Phani Motamarri (IISc)

Biography:

Vikram Gavini is an Associate Professor of Mechanical Engineering and Materials Science & Engineering at the University of Michigan. He received his PhD from California Institute of Technology in 2007. His interests are in developing methods for large-scale electronic structure calculations, numerical analysis of PDEs and scientific computing. DFT-FE, a massively parallel open-source code for large-scale DFT calculations, has been developed in his group. He is the recipient of the NSF CAREER Award in 2011, AFOSR Young Investigator Award in 2013, Alexander von Humboldt Foundation's Humboldt Research Fellowship for Experienced Researchers (2012-14), and the USACM Gallagher Award in 2015.

Innovation in Indian Science: Lessons from Covid-19

Vijay Chandru

Adjunct Visiting Professor, Centre for BioSystems Science and Engineering, Indian Institute of Science, Bangalore, India

Abstract:

Will this be an inflection point for Indian science and create a new cadre of scientists driven by a genuine interest in translation and impact in society? It would be difficult to answer such a sweeping question in the limitations of this talk. However, we shall examine a few anecdotes that suggest a movement in a positive direction prompted partly by the response to the pandemic but enabled by a foundation that has been laid over some time now – ever since the push for innovation in science and technology began to drive policy in 2010.

Biography:

Vijay Chandru had his formal training in Electrical Engineering (BITS, Pilani), in Systems Science and Engineering (UCLA) and in Decision Sciences (MIT). In today's nomenclature, he would be called an early data scientist. Building on this foundation, he had over 35 years of experience straddling various geographies, academic environments and industries. His academic career in teaching and research in computational mathematics was substantially at Purdue University (first 10 years) and the Indian Institute of Science with visiting appointments at University of Pennsylvania, Massachussetts Institute of Technology, and Stanford University. His departmental affiliations include Operations Research / Industrial / Systems Engineering, Computer Science and Business Administration.

Chandru is currently an adjunct visiting professor of interdisciplinary sciences in Bio-Engineering and in Cyber Physical Systems at the Indian Institute of Science.

Insights into unconventional ferroelectricity in hafnia-based systems through operando STEM and XRD.

Pavan Nakula

Professor, Center for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India

Abstract:

Hafnia-based thin-films have revived interest in ferroelectric devices and ferroelectricity in microelectronics. This is Si-friendly unconventional ferroelectricity, which becomes robust with miniaturization. Since 2015, in collaboration with different groups all over the world, my research has been focusing on primarily understanding this unconventional nature of ferroelectricity. This involved making epitaxial thin-films, their structure-property studies, and more recently trying to understand the ferroelectric switching in the devices through in-situ atomic resolution STEM (under bias, using an imaging technique called differential phase contrast) and operando nanobeam x-ray diffraction. The results from these experiments clearly showed that this ferroelectricity is extrinsic in nature, and heavily intertwined with oxygen vacancies and their migration. I will discuss the details of these findings in my talk and motivate that we should look at new material selection guidelines to explore this defect-based ferroelectricity in other simple oxide material systems. I'll also speak about some of the current work of my group in this direction.

Reference

P. Nukala et al., Reversible oxygen migration and phase transitions in hafnia-based ferroelectric devices, Science, 2021, Vol:372, pg: 630.

Biography:

Pavan Nukala is an Assistant Professor at the center for Nanoscience and Engineering, IISc Bangalore, India. He is a materials scientist by training. He did his bachelors and masters from IIT Madras in Metallurgical and Materials Engineering, PhD from the University of Pennsylvania. Later he was a post doc at University Paris Saclay, and a Marie Curie research fellow at the University of Groningen in the Netherlands. His research interests include understanding the physics of thin films and devices of various functional electronic materials including ferroelectric oxides, phase change materials, memristive and neuromorphic materials. His own expertise is on *in situ* atomic resolution microscopy and operando x-ray diffraction techniques.

Natural Materials - A Tale of Two Explorations

Vilupanur Ravi

Professor, Department of Chemical and Materials Engineering College of Engineering, Cal Poly Pomona, CA 91768, USA

Abstract:

Natural materials have inspired many innovations in engineering and science. In this talk, I will discuss two different examples. One of them will be about spider silk, a natural material that has unique mechanical properties, e.g., high strength-to-weight ratios. An introduction to the topic will be followed by a discussion of silk extraction, its properties and potential applications. In the second example, the materials science foundational to the construction of the plank canoe of the Chumash, a Native American people, will be discussed. This canoe, called the tomol, including the use of a material called yop. The yop, made from natural materials, functioned not only as a sealant and a caulking compound but also as an adhesive/binder. I will discuss the Chumash culture, the tomol, yop, and where it was utilized, and describe our efforts to process and characterize this material.

Biography:

Dr. Vilupanur A. Ravi is a Professor in the Department of Chemical and Materials Engineering at the California State Polytechnic University, Pomona (Cal Poly Pomona), USA. He is currently the K. P. Abraham Visiting Chair Professor in the Department of Materials Engineering at the Indian Institute of Science. He is an alumnus of the Institute, having obtained his B.E. in Metallurgy with distinction, followed by his MS and PhD from the Ohio State University. His IISc project, under the supervision of Profs. S. Ranganathan and K. Chattopadhyay, was awarded the Frank Adcock medal for the outstanding B.E. project, and led to a paper in Acta Metallurgica. Prof. Ravi’s research interests are in the areas of corrosion, high temperature materials/coatings and materials processing. His work has been recognized through several awards and honors both nationally and internationally including the NACE Technical Achievement Award, and Fellowships in seven different professional organizations including the National Academy of Inventors, ASM International, the American Association for the Advancement of Science, etc.

Platform Presentations

Rapid Blood Clotting with Silica/Silk Fibroin-Composite Based Bilayered Foam

Sushma Indrakumar[a], Santanu Ghosh[a], Tapan Dash[b], Vivek Mishra[b], Bharat Tandon[b], Kaushik Chatterjee[a]*

[a]*Department of Materials Engineering, Indian Institute of Science, Bangalore, India*
[b]*Fibroheal Woundcare Pvt. Ltd., Bangalore, India*

**E-mail* of corresponding author: *kchatterjee@iisc.ac.in*

Abstract

Uncontrolled bleeding caused due to traumatic injuries is a major cause of preventable deaths. Haemorrhage accounts for 40% of trauma mortality, 56% of which occur in the pre-hospital setting.1 In this scenario, researchers worldwide are trying to develop local haemostats that could induce rapid blood coagulation. In this study, we report a novel strategy by fabricating a bilayered hemostatic foam. Herein, the foam consists of a top bioactive layer (sub-micron sized silica particles (SPs)/silk fibroin composite); and a bottom thick chitosan foam. Although SPs and chitosan are strong procoagulants, they are mucoadhesive that could cause rebleeding during removal post-application.2,3 Therefore, SPs were loaded into a non-adhesive matrix (fibroin) to aid in easy removal while leaving its clotting behaviour unaltered. The second layer in the foam is a thick, porous chitosan foam that adds to the absorption capacity of the developed haemostat. To obtain the bilayered foam, a facile fabrication process of "two-step freezing and lyophilizing" was established. The foam composition was optimized based on the clotting behaviour of the individual components and the cytocompatibility. The haemostatic efficacy of the developed foam was compared with the recently FDA-approved product Axiostat. In the *in vivo* study, we demonstrate that the foam could achieve rapid haemostasis (30 s) with significantly lower blood loss ($p < 0.05$). Additionally, we address the limitations of adhesiveness and rebleeding, as is the case with Axiostat. Considering the ease of fabrication and hemostatic efficacy, the developed bilayered foam is envisioned as a successful hemostat used in pre-hospital hemorrhagic control.

References

1. Kauvar DS, *et al*., *Journal of Trauma and Acute Care Surgery*. **2006** Jun 1;60(6): S3-11.
2. Liu H, *et al*., *Particle & Particle Systems Characterization*. **2017** Dec;34(12):1700286.
3. Sogias IA, *et al., Biomacromolecules*. **2008** Jul 14;9(7):1837-42.

Exploration of NaSICON frameworks as calcium-ion battery cathodes

Dereje Bekele Tekliye and Sai Gautam Gopalakrishnan

Department of Materials Engineering, Indian Institute of Science

Abstract

The necessity of transition from fossil fuel to alternative carbon-free renewable energy sources results in an increased demand for energy storage devices like batteries, especially in electric vehicles, smart grids, and portable electronics. Lithium-ion battery (LIB) is the state-of-the-art energy storage technology due to its high energy and power density, good cycle life, and reliable performance. However, safety issues and high costs associated with the limited availability of raw materials (e.g., lithium and cobalt) casts uncertainty in fulfilling the future demand. As an alternative to LIB, where lithium ion (Li^{+1}) carries only one electrical charge, a possible pathway to increase the energy density is to switch to a multivalent (MV) ion-based battery chemistry that shuttle two (Mg^{2+}, Ca^{2+}, Zn^{2+}) or three (Al^{3+}) electrical charges at a time. Among MV systems, calcium ion battery (CIB) is an attractive candidate due to the low standard reduction potential of calcium (−2.87 V vs. standard hydrogen electrode), use of Ca - metal anode leading to high energy density, low cost, and abundance of Ca. The development of CIB technology is in its infancy due to the challenge of finding cathode materials that are electrochemically active and reversibly intercalating calcium ions. Using first-principles calculations, we perform a robust structural screening over the wide chemical space of sodium superionic conductor (NaSICON) frameworks, with a chemical formula of $Ca_xM_2(ZO_4)_3$ (where M = Ti, V, Cr, Mn, Fe, Co, or Ni, and Z = Si, P, or S). Specifically, we calculate the theoretical capacity, average Ca^{2+} intercalation voltage, and thermodynamic stability (at 0 K) of charged and discharged NaSICON compositions. We find that while all silicate-based Ca-NaSICONs are thermodynamically unstable and hence unsuitable as Ca-cathodes, several phosphate and sulphate-based Ca-NaSICONs appear as promising candidates as Ca-cathodes owing to their thermodynamic stability and Ca-intercalation voltage. We hope that our work will unearth a new pathway for developing practical CIBs.

Keywords: Calcium-ion battery; cathode materials; NaSICON

4D Printing of Multifunctional Biocompatible Magnetic Composites

Saswat Choudhary, Kaushik Chatterjee

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

Abstract

The field of 4D printing, which endows static 3D printed structures with the capability to transform their shapes over time, has gained much attention over recent years. This unique ability of shape transformation can be met by either use of smart materials and/or design principles to accurately program the printing paths. This work demonstrates excellent shape fixing, and shape recovery performances of 3D printed polylactide-co-trimethylene carbonate (PLMC). PLMC was 3D printed into simple 2D shapes and 3D scaffolds, both of which demonstrated excellent shape recovery ratios (close to 99%) at around 37°C. PLMC was further reinforced with magnetite nanoparticles, which can be responsive to alternating magnetic field stimuli due to the nanofillers' inductive heating ability. This can yield composites that can be remotely actuated via magnetic field to drive the shape recovery and, hence, be suited for various applications, including actuators, deployable scaffolds, etc. Both the polymers and composites were characterized for their thermal, chemical, and mechanical properties. The shape memory performances of the materials were quantitatively assessed by dynamic mechanical testing using cyclic test routines. In vitro biocompatibility of the materials was also evaluated using NIH 3T3 cells. Taken together, we developed a novel set of 4D printable materials which displayed good printability using extrusion printing, excellent shape recovery using remote actuation, and biocompatibility. These unique properties can render the materials useful for a variety of applications, including soft robotics, medicine, etc.

Investigation of thin-film delafossite materials for energy efficient memory devices

Suryakanta Mondal, Bhagwati Prasad

Department of Materials Engineering, Indian Institute of science

Abstract

In this era of artificial intelligence (AI) and the internet of things (IoT), there is an urgent need for low-power and high-speed non-volatile memory (NVM) solutions. Spin transfer torque (STT) based magnetic RAM (MRAM) emerged as a promising NVM technology. However, these devices operate at a high current, which creates a significant Joule heating effect on the circuit and thus damages the MgO barrier, which eventually decreases the device's endurance. In contrast, spin-orbit torque (SOT) memory devices operate at low input current besides the different read and write current paths, increasing switching speed and endurance. There is an urgent need for an energy-efficient SOT material. Delafossite materials are promising SOT materials as they possess excellent electrical conductivity (resistivity ~2.6$\boldsymbol{\mu}\Omega$cm) and show a large spin hall angle (>0.3). This project aims to investigate the thin film delafossite materials for energy-efficient non-volatile SOT-MRAM applications.

Keywords: Spin Orbit Torque (SOT), MRAM, STT, Spin Hall effect (SHE), Non-volatile memory (NVM), Internet of things (IOT)

Effect of Exchange-Correlation Functionals on the Estimation of Migration Barriers in Battery Materials

Reshma Devi, Baltej Singh, Pieremanuele Canepa, and Gopalakrishnan Sai Gautam

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

Abstract

Facile ionic mobility within-host frameworks is crucial in designing high-energy-density batteries with high-power densities, where the migration barrier (E_m) is the governing factor. This talk will discuss the accuracy and computational performance in calculated E_m, against experimental data, of several exchange-correlation (XC) functionals, within the density functional theory-nudged elastic band framework of six different electrodes and three diverse solid electrolytes. The generalized gradient approximation (GGA), the strongly constrained and appropriately normed (SCAN), and their Hubbard U corrections, GGA+U and SCAN+U, are the important XC functionals considered. It is observed that SCAN tends to be more accurate than other frameworks, albeit with higher computational costs and convergence difficulties, while GGA is a feasible choice for 'quick' and 'qualitative' E_m predictions. The sensitivity of E_m on adding uniform background charge and/or the climbing image approximation in solid electrolytes and the Hubbard U correction in electrodes are also quantified. This benchmarking will thus aid in selecting the suitable XC functional for a given structure in future studies, thus enabling the discovery of novel ion-conducting electrodes and solid electrolytes via computational workflows.

Keywords: Migration barriers; Exchange-correlation functionals.

Injectable and Self-Healing Polysaccharide-based Hydrogels for Sustained and Localized Delivery

Pritiranjan Mondal[1] and Kaushik Chatterjee[1]*

[1]*Department of Materials Engineering, Indian Institute of Science, C.V. Raman Avenue, Bangalore,India*

* E-mail of *Corresponding authors*: kchatterjee@iisc.ac.in Tel: +91-80-22933408

Abstract

The conventional injectable hydrogels without self-healing ability may be easily damaged by external forces which can deteriorate their functionalities. Therefore, self-healing injectable hydrogels, which can spontaneously restore the integrity of the network structures and functionalities after damage without the need for external interventions can be explored to meet the needs of biomedical applications. To address the emerging need for self-healing injectable hydrogels with improved functionality for the delivery of drugs, we designed a novel biocompatible and self-healing polysaccharide injectable hydrogel which have been formulated by dual crosslinking (chemical and ionic). These hydrogels exhibit outstanding viscoelastic, thixotropic, and self-healing characteristics, making them suitable for injectable drug delivery. MTT and Live /Dead assays revealed the non-cytotoxic nature of these hydrogels. Upon Doxorubicin and ciprofloxacin loading, these hydrogels demonstrated a sustainable release at physiological condition and drug-loaded hydrogels showed significant efficacy against cancer and bacterial growth. These formulated biodegradable and injectable hydrogels could find promising applications for the prolonged release of various drugs at the various sites in the body.

Micro-Texture Regions in Rolled Ti-6Al-4V Under Polarized Light

Faizan Hijazi[1], Dheepa Srinivasan[2], Barna Roy[1], Praveen Kumar[1] and Vikram Jayaram[1]

[1]*Department of Materials Engineering, Indian Institute of Science, Bangalore -560012 (India)*

[2]*Pratt & Whitney, Research and Development Center, Bangalore – 560012 (India)*

Abstract

Identifying micro-texture regions (MTR) in deformed Ti-6Al-4V requires extensive time in electron back-scattered diffraction (EBSD) imaging with a field of view that is limited to only a few millimeters. This study uses a novel method of high throughput identification of MTR using polarized light microscopy (PLM) and validation by correlation with orientation image mapping from EBSD. Reflection of polarized light under crossed polars leads to a difference in contrast depending on the orientation of the c-axis of the α-phase. MTR that are spread over a large area are visible in PLM as bands of contrast and the field of view is large compared to EBSD maps. It is shown that the shape and size of MTR may be captured accurately in PLM, and a one-to-one correspondence is demonstrated with such regions identified by EBSD with an excellent match between the area fraction of MTR calculated from both methods.

Keywords: Micro-texture; EBSD; polarized light microscopy

Gelatin-Sericin-Laminin Cryogels for Tissue Regeneration in Diabetic Wounds

Suhela. T,[1] Parvaiz A. Shiekh,[1] V. Verma[4,5], and A. Kumar.[1,3]

[1]*Department of Biological Science and Bioengineering, Indian Institute of Technology Kanpur,Kanpur, Uttar Pradesh 208016, India.*

[2]*Centre for Environmental Sciences and Engineering,*

[3]*Centre for Nanosciences, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh 208016, India, Centre for Environmental Sciences and Engineering,*

[4]*Centre for Environmental Sciences and Engineering,*

[5]*Materials Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh 208016, India.*

Abstract

Stem cell therapy presents a promising approach to achieve efficient healing in wounds like pressure ulcers, diabetic ulcers, venous ulcers, and arterial insufficiency ulcers. The healing cascade in such wounds is immensely hampered and causes both an economic burden and morbidity to patients. This may be attributed to a plethora of hostile conditions like elevated reactive oxygen species (ROS), impaired angiogenesis, senescent fibroblasts, and deficient stem cells that significantly diminish the probability of self-healing in these wounds. To address the complex scenario of chronic wounds, we propose a combinatorial approach of delivering ADSCs on antioxidant gelatin-sericin (GS) scaffolds coated with laminin (GSL), an endothelial basement protein to improve angiogenesis. The synthesized GS scaffolds showed values of compression modulus, pore size, porosity, and the swelling ratio in the range of 65 kPa, 158 ± 48.8 μm, 91.1% ± 1.25, and 28 ± 2.5, respectively. A DPPH assay revealed GS scaffolds exhibit around 20% more scavenging as against gelatin (G) scaffolds and better protection against free radical assault, thus enhancing cell viability and the metabolic index of fibroblast cells. Different cells, namely, fibroblasts, keratinocytes, and ADSCs, cultured on GS scaffolds had better metabolic activity as compared with G scaffolds. Laminin coating onto the scaffolds leads to improved attachment and tube formation of endothelial cells as depicted in scanning electron microscopy images. Finally, we validated the applicability of the ADSCs loaded laminin-coated GS scaffolds in a diabetic ulcer rat model. Hematoxylin and eosin, Masson's trichrome, and picrosirius red staining showed better regeneration and collagen remodeling in ADSCs loaded GSL scaffolds. Immunostaining of CD31 staining demonstrates enhanced angiogenesis in GSL-ADSC as compared with other groups.

Plasticity development and crack nucleation analysis under dwell fatigue loading of Ti 6242 by using ECCI

Tirthesh Ingale, Dipankar Banerjee

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

Abstract

Ti 6242 is a near alpha Ti alloy which is widely used in manufacturing turbine engine discs and blades. Because of ability of Ti alloys for room temperature creep, they undergo dwell debit at low temperature and high stresses. Unlike LCF, dwell fatigue crack nucleates at subsurface region. In spite of much work, mechanism for dwell fatigue crack nucleation in terms of operating slip systems is not completely understood. As, slip activity plays vital role in dwell fatigue, conventionally slip analysis in dwell fatigue is done by TEM. Because of size limitation, study of effect of each and every neighbour for crack nucleation becomes difficult. Alternatively, a SEM based technique 'Electron Channeling Contrast Imaging' (ECCI) has emerged which is capable of doing defect analysis for bulk specimen. Tensile tests were carried out for finding the YS and subsequently LCF and dwell fatigue tests were accomplished by different stress levels. Samples after the testing was thoroughly studied through SEM-EBSD coupled with ECCI techniques for slip analysis. The results explained the evolution of differentslip systems, slip transfer and the difference in plasticity development during different loading conditions.

Keywords: Ti alloy, Dwell Fatigue, LCF, ECCI

Ballistic impact failure characteristics of Al 2024-T351

Sazid Khan, S. Karthikeyan

Department of Materials Engineering, Indian Institute of Science, Bangalore, 560012

Abstract

Dynamic failure analysis of materials is important in applications such as penetration resistance of defense armors, automotive crashworthiness, prevention of the catastrophic failure of pressure vessels, and aircraft burst containment. The mode of failure of a material varies with its thickness and the projectile's size, shape, and velocity. Therefore, it is crucial to understand the complete description of the material behavior under impact loading to mitigate these risks. Experimental approaches have constraints on cost, time, and repeatability for several possible scenarios. In contrast, numerical modeling is free of such constraints. However, one of the limitations in numerical modeling is the availability of an accurate ductile failure model that can correctly predict the failure modes during impact loading. The present work was done to shed light on the phenomenological ductile failure model of Al 2024-T351 alloy under ballistic impact. Al 2024-T351 is widely used in aircraft structures due to its high strength-to-weight ratio and fatigue resistance. The ballistic impact experiments (ball impact on a plate) were carried out on a 1.45 mm thick Al 2024-T351 target with a 6 mm diameter ball. Constant fracture strain, Johnson–Cook, and generalized incremental stressstate-dependent (GISSMO) damage models were used in a finite element framework to predict the ballistic characteristics of Al-2024-T351. A strong correlation between experiments and simulation results was found with the GISSMO model.

Keywords: Ballistic Impact; Johnson–Cook; GISSMO

An investigation of multiphase flows through a packed bed with implications to iron-making blast furnaces

Ferdin Sagai Don Bosco, Govind S. Gupta

Materials Engineering, Indian Institute of Science, Bangalore.

Abstract

The complex, multiphase flow inside an iron-making blast furnace relies on the permeability of the coke bed for operational stability and productivity. Permeability is adversely affected by the accumulation of unburnt coal and coke powder resulting from Pulverised Coal Injection (PCI) and the presence of fused iron in the cohesive zone. Liquid iron and slag percolate from the fused iron blocks and flows as rivulets and droplets through the packed coke bed. Achievement of a stable operation at high PCI rate necessitates a deeper understanding of the distribution of gas, liquid and powder flows due to a reduction in permeability, the effect of the cohesive zone on raceway, and powder accumulation characteristics in the blast furnace. A computational study of a laterally injected gas-powder flow through a tuyere, which protrudes into a two-dimensional packed bed in the presence of raceways and cohesive zones is undertaken in this research. The gas and powder phases are modelled as a two-fluid system which are closed by appropriate interphase force models. The packed coke bed and the evolution of the raceway shape and size are replicated through a discrete element method (DEM), wherein the motion of individual particles are governed by Newton's law. A correlation, based on experimental data, is used to predict the static portion of the accumulated powder. An in-house solver is developed and the results indicate an excellent agreement with the experimental data, which lends credibility to the model and solver. The effect of operational parameters such as gas flow rate, particle size and density, and, powder feed rate and size are analysed. Additionally, structural parameters such as cohesive zone configuration, block porosity, and tuyere protrusion are also varied, and their effect on the raceway and static holdup profiles are characterised. The sensitivity analysis shows that the raceway shape and size and interaction with the cohesive blocks play a vital role in the distribution and accumulation of powder.

Keywords: Multiphase flow simulations, Pulverized coal injection, Blast furnace modelling, lateral injection, Raceway characterization, powder accumulations, discrete liquid flows

Design of a polymer encapsulating film to prevent lead leakage from lead perovskite solar cells

Jinu Joji, Praveen C Ramamurthy

Department of Materials Engineering, Indian Institute of Science, Bangalore

Abstract

Lead halide perovskite, it is a highly efficient active material among the perovskite solar cell family. The degradation of lead halide perovskite and leaching of lead is hazardous. Several methods have been developed for the lead mitigation approach which includes Encapsulation with glass and polymer, in situ regeneration lead halide, etc. Effect of encapsulation on the stability of perovskite as a moisture barrier has been explored. Hence, extending the use of encapsulants in a way to prevent the leaching of lead from the solar cell is a practical approach. Modification of existing polymer encapsulants with lead capturing molecules is promising. Here, in this work a polymer film is modified by surface polymerization of polydopamine (PDA) followed by the incorporation of ZIF- 67. The modified ZIF- 67- PDA- polymer film was shown a 7-fold decrease in the lead leakage compared to neat polymer film. Therefore, the modified polymer film can be used as an effective encapsulant to prevent lead leakage from lead perovskite solar cell.

Keywords: Polymer, Lead, ZIF- 67, PDA

A phase transformation in steel during hot deformation: unique features revealed through crystallographic texture

B. Aashranth[1,2], Dipti Samantaray[2], Satyam Suwas[1]

[1]*Indian Institute of Science, Bangalore, India*

[2]*Metallurgy and Materials Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, India*

Abstract

High temperature deformation, in several steels, under specific conditions, results in the conversion of austenite to ferrite, even above its usual stable temperature. This phenomenon has been referred to by several names and is the subject of considerable debate and divergence. While some aspects of the transformation have been unequivocally accepted, others remain areas of active research. These include the mode of transformation; whether diffusional, massive or displacive, as well as the specific conditions that enable such transformation. It is not clear which component of hot deformation causes the transformation; the plastic strain imposed, or the stress. This difference, as addressed in the current work, is crucial from a fundamental as well as technological standpoint. The ambiguities associated with this transformation are critically assessed through the lens of crystallographic texture. It is shown that the deformation/transformation textures show distinct signatures that help reveal the mode and mechanism of this unique phase transformation.

Keywords: EBSD, steel, phase transformation

Direct energy deposition of a low modulus TNZT alloy for biomedical applications

Saurabh Kumar Gupta[1], Kaushik Chatterjee[1], Satyam Suwas[1]

[1]*Department of Materials Engineering, Indian Institute of Science, Bangalore, India*

Abstract

Additive manufacturing of metals and alloys offers a unique route for preparing customized implants. Direct energy deposition (DED) is one of the additive manufacturing processes that can yield patient-specific implants. TNZT, a β-type titanium alloy, exhibits a combination of excellent biocompatibility, high strength, good corrosion resistance and low elastic modulus. Additive manufacturing of TNZT by DED has received little attention in the scientific literature. Gas atomized Ti-34Nb-7Zr-5Ta powder was used for DED in this study. Design of experiment (DOE) was performed by varying key parameters such as power, scanning speed, rotation between layers and powder flow rate. Parameter optimization study was performed and at optimized parameters nearly dense component was produced. Defects such as lack of fusion, cracks and spherical porosity was observed in several conditions. By increasing the power, lack of fusion was completely removed, and nearly dense components were produced. Qualification of these dense components were studied through microstructural analysis, crystallographic texture and mechanical behaviour study. X-ray diffraction analysis was carried out for structural characterization, and it showed the presence of β phase only. Micro-hardness measurement was done, and it did not show anisotropy along the build direction. However, small change in micro-hardness between two dense conditions was observed. Increase in power during fabrication of components resulted into stronger texture formation along build direction. These results have important implications for preparing the next generation of orthopedic implants.

Keywords: Additive Manufacturing, Titanium Alloys, Biomedical Implants

Role of characterisation techniques in understanding the microstructure of metal additive manufacturing

Deepak Kumar[1], Soumita Mondal[1], KG Prashanth[2,3,4], Satyam Suwas[1]

[1]*Department of Materials Engineering, Indian Institute of Science, Bangalore*

[2] *Department of Mechanical and Industrial Engineering, Tallinn University of Technology, Ehitajate Tee 5, 19086, Tallinn, Estonia*

[3] *Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A8700 Leoben, Austria*

[4] *CBCMT, School of Mechanical Engineering, Vellore Institute of Technology, Vellore, Tamil Nadu, India*

Abstract

Metal additive manufacturing (AM) has emerged as a research hotspot recently. Looking to the future, it can be confidently predicted that AM is set to achieve an increasing market share of production processes, helped with the introduction of faster systems with more powerful lasers and larger building chambers. A significant number of materials will be qualified for AM and over time multi-material systems for many of the processes will become available. Understanding of the various phenomena in AM requires an awareness for plausible usability of available characterisation techniques. This presentation shows various applicable metallurgical techniques to characterize materials, role of processing effects, and post-deformed generated structures in metal AM. Macro-, meso-, micro- and nano-scale characterization of the internal structure will be presented to show how various techniques can be specifically utilized to better understand the materials and processing conditions and their effects on the performance of these materials for various applications. Materials covered would be selectively laser melted stainless steel 316L, Cu based alloy and Al-Si-Mg.

Keywords: AM; characterisation; ECCI; EBSD; X-ray tomography; APT

Understanding creep deformation behavior of extruded Mg-Ce alloys

Hemant Kumar, Surendra Kumar Makineni

Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

Abstract

Light-weight Mg alloys attract great attention for automotive applications, especially in power train components. Ce is a promising alloying addition to improve the mechanical properties at room and high temperatures. However, their role is not clearly understood. In the present work, the creep deformation behavior of extruded pure Mg and Mg-0.5 wt.% Ce alloys is studied under compressive loading. The microstructural analysis of the alloys before and after creep is studied using Optical Microscope (OM), Scanning Electron Microscopy (SEM), Electron BackScattered Diffraction (EBSD), Transmission Electron Microscopy (TEM), and Atom Probe Tomography (APT). The results highlight the role of Ce and its effect on the deformation behavior of the alloy. TEM and APT reveals Ce segregation at the interfaces, such as grain boundaries and creep-induced micro-twins. The obtained results are discussed based on the measured creep properties of the alloy.

Keywords: Creep Deformation, Ce-segregation, Twins, HAADF-STEM, APT.

Controlled electron channeling contrast imaging of defects in engineering alloys

Akshat Godha, Surendra Kumar Makineni

Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

Abstract

Electron channeling contrast imaging (ECCI) enables observation and quantification of crystalline defects in bulk samples. This work shows the combined use of TSL OIM and Single Crystal (S.C.) Softwares that guided to obtain channeling contrast from the surface of the samples. The former gave the exact orientation of grain at the surface, while the latter was used to simulate the corresponding electron channeling pattern (ECP). A set of rotation and tilt angles for two-beam conditions were calculated from the simulated ECP in SC software. Subsequently, the microscope stage was positioned accordingly, and ECC images were captured from the region of interest in the samples. This is demonstrated for dislocations, stacking faults, twins, and low angle grain boundaries in several metallic engineering alloys.

Keywords: ECCI, TSL OIM, SC, Dislocations, Stacking Faults, Twins.

Engineered nanotopography on 3D-printed polymer scaffolds to impart mechanobactericidal property

Deepak Patil, Kaushik Chatterjee

Department of Materials Engineering, Indian Institute of Science, Bangalore, 560012, India

Abstract

Bone is one of the most widely transplanted tissues of the human body. With increasing lifespan and incidences of lifestyle diseases, aside from trauma and congenital disorders, there is an ever growing demand for bone tissue engineering. A three-dimensional (3D) biodegradable scaffold that serves as a temporary construct is essential to facilitate new tissue growth at the defect site. However, the recurrent implant-associated infection due to bacterial attack at the surgical site puts an enormous clinical and economic burden, especially with rising cases of antimicrobial resistance. Infection at the surgical site arises as bacteria penetrate the defect site during a surgical procedure and colonize the biomaterial surface, which has been a significant problem in orthopedic surgery. Implant-mediated infections can become resistant to antimicrobial agents are ineffective, and implant removal becomes the last option that may put the patient's life at risk. Bioinspired nanotopography similar to the nanopillars on some insect wings motivated the fabrication of biomimetic bactericidal nanostructures on biomedical devices. This study aims to develop scalable surface modification processes capable of producing bactericidal nanotopography on 3D biodegradable polymer scaffolds. The goal was to physically alter the surface topography of the as-printed 3D polymer scaffold to make it effective against a wide range of bacteria without using chemical agents. The nanotopography significantly inhibited the growth of E. coli and S. aureus, as revealed by live/dead fluorescence images. This is attributed to the nanopillars fabricated on the scaffold surface that physically rupture the bacterial membrane. Hence, the leaching-free, antibacterial, and biocompatible polymer scaffolds can be directly employed bone tissue regeneration.

Keywords: Biomimicry, Nanotopography, Spin coating, Bactericidal property.

3D Bioprinting of Photo-crosslinkable Kappa-Carrageenan to Fabricate Cell-loaded Tissue Scaffolds

S. Kumari[1], P. Mondal[1], and K. Chatterjee*

[1]*Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India*

Abstract

Digital light processing (DLP) printing technology enables the rapid fabrication of complex three-dimensional (3D) cell-laden structures for tissue engineering, and in-vitro models for drug testing applications. Here, we demonstrate the outstanding printability of photocurable methacrylate-κ-carrageenan (MA-κ-CA) using DLP printing. The MA-κ-CA printing precursors were synthesized by covalent grafting of methacrylate moieties to the hydroxyl functional groups of κ-CA with a high degree of substitution (DS) of 48 %. 3D printed hydrogels with varying concentrations of 1, 2, 3, 4 and 5 % (w/v) of MA-κ-CA were produced within minutes with a curing time of 5 s per layer and were thoroughly investigated for properties of swelling, degradation, mechanical, rheology, and suitability for bioprinting with living cells. Viscosity and shear thinning behavior of MA-κ-CA are optimal for the bioprinting of cells. The resulting data for 3D printed structures with NIH 3T3 and HaCaT cells show high viability as well as proliferation over days with enhanced shape and structural integrity of hydrogels. Furthermore, through the DLP printing of MA-κ-CA, highly complex 3d hydrogel scaffolds were printed with high accuracy, and resolution to implement the biological complexity in the bioprinting of tissues and organs.

Keywords: digital light processing, carbohydrates, 3D bioprinting

Poster Presentations

Graphene oxide-functionalized metal organic framework naphthalene dicarboxylic acid (UiO-66-NDC) as a novel adsorbent for the removal of As (V) from aqueous solutions

Simranjeet Singh[1], TS Sunil Kumar Naik[2], S. Subramanian[2], and Praveen C Ramamurthy[1,2]

Corresponding author: praveen@iisc.ac.in

[1]*Interdisciplinary Centre for Water Research (ICWaR), Indian Institute of Science, Bangalore, India*

[2]*Department of Material Engineering, Indian Institute of Science, Bangalore-560012*

Abstract

The present study deals with the synthesis of a hybrid nano-adsorbent through the intercalation of graphene oxide (GO)and metal organic framework naphthalene dicarboxylic acid (UiO-66 NDC). The synthesized hybrid adsorbent was characterized by X-ray powder diffraction (XRD), Raman spectroscopy,UV-visible spectrophotometry, scanning electron microscopy (SEM), Fourier Transform Infrared spectroscopy (FTIR),and Brunauer-Emmett-Teller (BET)surface area analysis. It was observed that UiO-66 NDC/GO shows better adsorption capacity and removal efficiency of As (V) at pH 3. The adsorption kinetics data followed pseudo-second-order model (Type 2 & 3), indicating that the adsorption process of As (V) is by chemisorption. The adsorption data was fitted to all the three isotherms, namely Langmuir, Freundlich and Temkin, though the Langmuir model had the best fit (R20.978), indicating the adsorption process occurred on the monolayered structure. The maximum adsorption capacity of As (V) was found to be147.1mg/g at room temperature(25°C). Thermodynamic parameters ΔH° and ΔG° were found to be negative confirming that the As(V) adsorption process was exothermic and occurred spontaneously. UiO-66-NDC/GO also showed high reusability for upto six regeneration performances using 0.01 M HCl as are generant. This is the first report of an MoF nanocomposite employed as a super nano-adsorbent for As (V) removal from simulated wastewater samples.

Keywords: GO/UiO-66-NDC; As(V); adsorption; Isotherms: Kinetics modelling

Facile and rapid sprayable conducting coating with stable conjugates of graphene nanoplatelets and carbon nanotubes for anti-corrosive applications

Sandeep Tripathi[1], Om Prakash[2], Devansh Sharma[1], Jagadeshvaran P L[1], Kamaraj. K[2], Suryasarathi Bose*[1]

[1]*Department of Materials Engineering, Indian Institute of Science, Bengaluru-560012, India*

[2]*Boeing, India Pvt Ltd, M.S Ramaiah Institute of Technology, MSR Nagar, Bengaluru- 560054, India.*

Abstract

Multifunctional polymeric coatings with superior surface conductivity and anti-corrosive properties are in high demand. Herein, stable conjugates of graphene nanoplatelets (GNP) and multiwalled carbon nanotube (CNT) were designed by non-covalently functionalizing the individual entities with Pyrene butyric acid (PBA). Such conjugates were stable and are spray-able over large substrates (both conducting and non-conducting). The chemical conjugation improved the dispersion stability and compatibility with the binder. This stable suspension when sprayed over various substrates like metal and non-conducting substrates like PET, glass etc., resulted in uniform coatings that are highly conducting. The surfaces are hydrophobic in nature as revealed from the water contact angle measurements. When coated over metals, the corrosion resistance behavior of PBA-CNT and PBA-GNP, estimated using potentiodynamic techniques, was excellent wherein, the conjugates act as an effective blockade against aggressive oxidant species.

Keywords: CNT, GNP, surface conductivity, anti-corrosive coatings

Sustainable nanosheet membranes derived from graphene oxide stitched dense ‘covalent organic framework’ for effective water remediation

Sk Safikul Islam, Subhasish Maiti, Suryasarathi Bose*

Department of Materials Engineering, Indian Institute of Science, Bangalore, Karnataka-560012, India.

Abstract

2D materials like graphene oxide (GO) based free-standing membranes though have shown excellent salt rejection at short time scales but suffer from structural stability and swelling on prolonged usage. Hence, in this study, a unique approach of crosslinking GO sheets with dense ‘covalent organic framework’ (to yield GO@COF) was designed to selectively reject ions and dyes. The GO@COF membrane was supported on a porous crystalline support (here polyvinylidene difluride, PVDF) designed by etching out the amorphous phase (here polymethyl methacrylate, PMMA) from demixed crystalline/amorphous pair. This arrangement showed good water flux, fouling resistance, and >90% dye rejection. In order to enhance the rejection further and improve the chlorine tolerance of the membrane, COF embedded polyamide (PA) thin-film composite membrane was designed in-situon this highly stable, non-swellable GO@COF membrane. This modified membrane showed excellent salt (>94% and >98% for monovalent and divalent ions, respectively) and dyes (>99.90% for both cationic and anionic dyes) rejection and in addition, demonstrated excellent resistance to fouling (>93%). Moreover, this sandwich structure revealed outstanding chlorine tolerance performance, thereby addressing the most significant challenges faced by either 2D materials-based or thin-film composite membranes.

Keywords: 2D materials; covalent organic frame work; desalination; chlorine tolerance

Stimuli-Responsive bio-inspired sequential interpenetrating polymeric membranes for efficient antibiotic and dye removal application

Ria Sen Gupta, Nagarajan Padmavathy, Piyush Agarwal and Suryasarathi Bose*

Department of Materials engineering, Indian Institute of Science, Bangalore -560012

Abstract:

A mussel-inspired membrane was engineered using an interpenetrating polymeric network (IPN) and was used to target antibiotics and pH-responsive dye removal with a rigorous and speedy reaction. Through charge and pore-based screening, these mechanically durable and environmentally sustainable membranes were made selective and effective towards certain dyes and antibiotics. In limited nanoscale regions, such molecular architecture resulted in unique chemical interactions, which facilitated separations. Various spectroscopic and microscopic techniques, as well as zeta potential, TGA, and water contact angle measurements, were used to characterise the final pore designed membrane. Over multiple cycles of operation, it was able to reject >97 percent of both Methylene blue (cationic dye) and Congo Red (anionic dye) at diverse pH conditions. Furthermore, it has the potential to eliminate over 96 percent of both Amoxicillin and Azithromycin medicines. This bioinspired pore-engineered IPN designed membrane is cost-efficient, resilient, stable, non-cytotoxic, and effective in separating antibiotics and organic dyes, making it a promising choice for water remediation.

Keywords: bio-inspired, pH-responsive, interpenetrating polymeric network, antibiotic removal, dye rejection, membranes, water-scarcity, Amoxicillin, Azithromycin

pH Triggered Carbon Nanotube Nanolaminates on Interpenetrating Polymer Network for Electromagnetic Interference Shielding Application

Kunal Manna, Ria Sengupta, Suryasarathi Bose

Department of Materials Engineering, IISc Bangalore, Bengaluru – 560012, India

Abstract

While both the usage and miniaturization of electronic gadgets have become quite imperative in the modern era, the factors (like stray electromagnetic signals) that affect their reliability also has attracted prime attention. In this context, lightweight and high-speed electronic gadgets need solutions that are ultra-thin, robust, sustainable, easy to integrate, and more importantly, are reliable. Herein, a construct is designed through pH-responsive self-assembly of carbon nanotubes (CNTs) on a sequential interpenetrating polymeric network (IPN) membrane. The charge on the IPN membrane can be triggered to facilitate the self-assembly of oppositely charged CNTs and this phenomenon can be switched. The shielding performance (> 300 dB/mm in a wide frequency band, 8.2-26.5 GHz) of this ultra-thin (~150 microns), light-weight CNT laminate nearly remained the same when subjected to 10,000 bending cycles. Such facile strategies can yield robust, sustainable, and easy-to-integrate solutions to this challenge.

Keywords: IPN, Carbon Nanotube, Nanolaminate, EMI Shielding

Microstructural and texture investigation on shock wave assisted deformation of Cp-Titanium

Shreshtha Ranjana[a], Gopalan Jagadeesh[c], Satyam Suwas[b]

[a]*Interdisciplinary Centre for Energy Research, Indian Institute of Science, Bangalore, India*

[b]*Department of Materials Engineering, Indian Institute of Science, Bangalore, India*

[c]*Department of Aerospace Engineering, Indian Institute of Science, Bangalore, India*

Abstract

Explosive/Blast forming is used for high velocity frictionless forming of thin sheets into complicated shapes. The purpose of present work is to study the microstructural and texture changes under the high strain rate deformation like shock/blast loading for commercial pure titanium. Titanium alloys are widely used in aerospace application due to its high strength to weight ratio. The possibility of shock forming of cp-titanium is observed. Bulk texture and microstructural analysis are carried out. There is significant weakening of bulk texture is observed because of grain fragmentation which produces many new orientations and leads to grain refinement. Deformation twinning which was seen in the after-shock microstructure also play role in texture weakening. The initial grain size distribution of annealed titanium is 84±20$\mu m$and after shock deformation it reduced to 15±8μm. Aspect ratio of grain changed from equiaxed to 3:1 along the shock direction after deformation. Formation of extensive deformation twins (15.2%) occur after deformation. $\langle\bar{1}010\rangle$ 64.4Ocontraction twin (CT1) is dominant resulting the splitting of basal poles toward the TD of (0002) pole figure. Strain gradient within the grain having higher value at the grain boundary can be seen. Microhardness was found to be highest at the mid-point defection region and it decreases systematically toward the periphery in deformed cp titanium.

Keywords: Titanium; Microstructure; Texture; Shockwave; High strain rate

Micromechanical response of commercially pure titanium Insights from experiments and simulations

S Tejanath Reddy, K.U. Yazar, Satyam Suwas

Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

Abstract

A microstructural patch of polycrystalline commercially pure titanium obtained through Electron Back Scattered Diffraction (EBSD) was used to study the slip activity, heterogeneous stress distribution, and texture evolution during uniaxial tensile deformation through a combination of experiments and crystal plasticity fast Fourier transform (CPFFT) simulations. The differences in the above-mentioned aspects while deformed along the rolling and transverse directions were studied. A higher strain hardening was observed when deformed along the rolling direction when compared to the transverse direction which was attributed to the higher activity of prism slip. While a texture component with RD || $\langle 10\bar{1}0\rangle$ was observed when deformed along rolling direction, a component in between $\langle 0001\rangle$ and $\langle 10\bar{1}0\rangle$ was observed for transverse direction loading. It was observed that some of the grains developed higher amount of stress post-deformation. These locations are termed as stress hotspots which interestingly was observed to be higher when deformed along rolling direction. These hotspots, irrespective of the loading direction had a similar initial orientation. The presence of large number of grains with this orientation resultedin the higher number of stress hotspots in rolling direction samples.

Keywords: Commercially pure titanium, EBSD, CPFFT, DAMASK.

On the effect of Al and Ti addition on microstructure evolution in NiCoCr multicomponent alloy

S. Sarang, Nithin Baler, Surendra Kumar Makineni

Department of Materials Engineering, Indian Institute of Science, Bangalore-560012

Abstract

Alloying and Thermo-Mechanical processing (TMP) is an effective way of tailoring the microstructure and mechanical properties of engineering alloys to overcome the strength ductility tradeoff. In this work, we explored the effect of Al, Ti addition and TMP (cold work + Annealing) on the microstructure and mechanical properties of NiCoCr multicomponent alloys. TMP followed by annealing at 700 °C for 20 hrs results in the formation of fine FCC grains with lamellar type of discontinuous precipitates. Transmission Electron Microscopy (TEM) and Atom Probe Tomography (APT) analysis revealed the discontinuous precipitates are of L12 type (ordered) with a stoichiometry (Ni, Co)3(Al, Ti). The composite microstructure results in a 0.2 % proof strength value of 1075 ±10 MPa, ultimate tensile strength of 1390 ±15 MPa with 28±3 % elongation till fracture. The investigation of deformed samples revealed the formation of stacking faults (SF), deformation twins (DT) (which is responsible for higher work hardening rate (WH)) and shearing of L12ordered precipitates (responsible for higher strength).

Keywords: Multicomponent alloys, Thermomechanical processing, Work Hardening Rate.

3D Bioprinting of Hydrogels for Studying Breast Cancer

Sriram Bharath Gugulothu, Kaushik Chatterjee

Department of Materials Engineering, Indian Institute of Science, Bengaluru, India – 560012

Abstract:

Breast cancer is a leading form of cancer in women, and by 2050 it can be a leading cause of cancer-related deaths. Triple-negative breast cancer represents the most aggressive form of breast cancer with poor prognosis. Current strategies to treat triple-negative breast cancer are limited, and immunotherapeutic strategies like targeting tumor-associated macrophages whichare not very successful in clinical trials that underscore the development of clinically relevant 3D in vitro models for better understanding and novel drug development towards breast cancer tumor metastasis anti-tumor associated macrophage immunotherapeutics. 3D bioprinting can address this issue compared to conventional approaches like a scaffold-based 3D model by incorporating multiple cell types along with spatial patterning of cells in a high throughput manner with tissue-specific stiffness to recreate tumor microenvironment complexity. In the current research work, a co-culture model for triple-negative breast cancer and monocytes will be developed using extrusion-based bioprinting to understand the epithelial to mesenchymal transition of cancer cells and monocytes polarization towards tumor-associated macrophages during their co-culture. To achieve this, an alginate and gelatin-based bioink was developed and characterized for physicochemical and rheological properties, followed by 3D bioprinting parameters optimization for individual or both MDA-MB-231 (triple-negative breast cancer cell line) and THP1 (monocyte cell line) cells at different cell density and further monitored cell viability, proliferation, and morphological features of cells in 3D for 14 days. EMT-specific markers like vimentin immunocytochemistry were performed for 2D vs. 3D bioprinted cell-laden constructs of MDA-MB-231 cells. Further, a paracrine and juxtracrine model for THP1 and MDA-MB-231 cells will be developed to understand the cellular level crosstalk through relevant phenotypic characterization for EMT, macrophage polarization specific gene and cytokines expression analysis in individual vs. co-culture models to evaluate the relevance of the 3D model and its applicability for drug screening of immunotherapeutics.

Investigation of Spintronics devices for energy-efficient non-volatile memory solutions

Naveen Negi, Astha Khandelwal, Suryakanta Mondal, Bhagwati Prasad

Department of Materials Engineering, Indian Institute of Science, Bengaluru

Abstract:

In this era of artificial intelligence (AI) and the internet of things (IoT), there is an urgent need for low-power and high-speed non-volatile memory (NVM) solutions. As of now, the memory and storage devices in the current computation architecture are either volatile or have high latency, or even consume high power, and therefore not suitable for handling the upcoming storm of big data. Moreover, the scaling of the conventional CMOS based technology below 7 nm has become challenging due to the unavoidable power losses in terms of heat, the complexity of the device fabrication processes, and the involvement of the quantum effect at that length scale. Over the last decade, several beyond-CMOS computing and memory technologies have been investigated to address these challenges. Among them, spintronics-based devices have emerged not only promising NVM solutions but also becoming alternative logic systems for in-memory and neuromorphic computing applications. Magnetic Random-Access Memory (MRAM) is a core element of prominent spintronic devices, where several mechanisms have been conceptualized to manipulate the resistance states of MRAM devices. The spin-transfer torque (STT) technique is being mainly used in state-of-the-art MRAM technology; however the issues of high switching current, low endurance, and lower tunnel magnetoresistance (TMR) response of these devices limit its application for standalone memory. To address these issues, we are exploring several novel concepts, such as Spin-Orbit Torque (SOT), Voltage-Controlled Magnetic Anisotropy (VCMA), and magnetoelectrics to modulate the resistance state of MRAM devices. We are investigating various materials systems to realize this purpose, such as: delafossite oxides for SOT, multiferroic oxides for magnetoelectric, and 2D ferromagnetic systems for VCMA. We grow the thin films of these materials and subsequently fabricate the spintronics devices and finally perform the magneto-transport measurements. Our efforts will provide several pathways to realized energy-efficient NVM solutions for AI and IoT applications.

Keywords**:** Spintronics, Artificial Intelligence, Internet of Things, Non-volatile memory, MRAM, Beyond-CMOS

Development of 3D in vitro model for anti-fibrotic drug testing for liver fibrosis

Piyush S. Agarwal[1], Shervanthi Homer-Vanniasinkam[1,2], Kaushik Chatterjee[1]*

[1]*Department of Materials Engineering, Indian Institute of Science, Bangalore, India 560012*
[2] *Department of Mechanical Engineering, University College London (UCL), Torrington Place, London WC1E 7JE, UK*

Abstract

Obesity is a serious global problem and has affected millions of people and the numbers continue to increase. Fatty Liver is an important cause of liver disease and approximately 30% of the general Indian population suffer from fatty liver issue and the prevalence is higher in those with overweight or obesity and with diabetes or pre-diabetes. Since there is very limited option to recover from fatty liver, e.g., diet modification and exercise, the fatty liver progress to liver cirrhosis and liver carcinoma.

Since research groups worldwide are trying to develop new therapeutic efficient options for the treatment, there is requirement for robust drug testing platforms. The traditional method is to test a drug is by evaluating the response of cells in 2D (two dimension) culture, animal model, and then human clinical trials. 2D culture and animal physiology do not mimic human physiology. Consequently, many drugs fail in clinical trials. This causes delays and increases research costs and few drug candidates are successful in human trials. Thus, there is an enormous demand for 3D (three dimension) in vitro models to evaluate the drug efficacy that can faithfully mimic human physiology before clinical trials.

Our aim is to mimic diseased liver physiology in vitro using three dimensional (3D) bioprinting of liver cells. 3D bioprinting helps in precise special arrangements of parenchymal and non-parenchymal cells and thus a better possibility to develop liver physiology. For this purpose, we have used alginate and gelatin hydrogel to prepare a bioink by mixing HepG2/Lx2 cells. We performed physico-chemical characterization to evaluate material's mechanical properties and biological characterization to evaluate its biocompatibility. To evaluate its the functional properties of the two cells in 3D, gene expression and synthesis of albumin will be quantified using RT-PCR and immune histochemistry.

Next generation thermoplastic laminates with tailored interfaces for aerostructural applications

Rishi Raj, Subodh Kumar, Suryasarathi Bose

Department of Materials Engineering, Indian Institute of Science, Bangalore, India 560012

Abstract:

The use of carbon fiber reinforced polymers (CFRPs) in the form of epoxy/carbon fiber (E/CF) laminates in the aircraft structures is a five-decade old technological advancement with current share of more than 50% by weight Boeing-787 and Airbus. They are widely used in primary structures of aircrafts such as wing panels, fuselages as well as secondary structures like tail parts, pylon skins etc. However, E/CF laminates have some unavoidable challenges such as the low damage tolerance, catastrophic brittle failure of the structures, property deteoriation due to prolonged aero-frictional/engine heat during service and huge production cost and time. To overcome these challenges, aromatic thermoplastics such as Polyetheretherketone (PEEK), Polyetherketoneketone (PEKK), Polyphenylenesulfide (PPS) and Polyetherimide (PEI) are becoming a popular candidate to replace epoxy in the CFRP laminates. The PEEK /CF composite laminates have very high strength (10 times damage tolerance than E/CF) and can sustain prolonged high temperatures (up to 250oC) exposures. The other mechanical properties (ILSS, Flexural strength) and flying qualification properties of PEEK/CF are comparable to E/CF. In spite of several advantages with the PEEK/CF laminates, the smooth surface of CF, lack of functional groups, mismatch in surface energies of PEEK and CF are responsible for weak interfaces between PEEK and CF. Several attempts have been made in the past to increase the interfacial adhesion between PEEK and CF which includes ozone, plasma, laser, and acid treatment to impart functional groups and surface roughness. However, the improvement in the properties (ILSS and flexural strength) is not significant due to damage to CF surface. Also, the functionalization process is a multi-step and long process which lacks industrial scalability. This work proposes to use low molecular weight aromatic polymer as a coating (sizing agent) over CF for improving interfacial adhesion with PEEK matrix. The sizing agents containing aromatic and functional groups are miscible with the PEEK matrix and can interact through π- π and polar interactions.

Keywords: CFRPs; Thermoplastic laminates; Interface; Sizing agent

Synergistic effect of external magnetic field on initiation of crack propagation in pre-cracked current-carrying Al foil

Swanand Telpande[a], Shubham Jain[b] and Praveen Kumar[c]

[a,b,c] *Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India*

[a]*Email id: swanandt@iisc.ac.in*

Abstract:

Applications such as microelectronic systems, integrated circuits, electromagnetic devices experience electrical surges of very high current density, of the order of 109A/m^2, during their service. The structural integrity of such components is a concern as flaws can propagate due to such high current densities. These components also experience the magnetic fields of the other surrounding conductors, which may enhance the severity of the electromagnetic forces. In this study, we have investigated the effect of the external magnetic field on the fracture behavior of pre-notched current-carrying Al foil. Experiments were carried out using a custom-built setup wherein current pulses were passed through the foil in presence of a uniform external magnetic field. The effect of increasing magnetic field on the critical current density required to initiate crack propagation was determined through these experiments. Numerical analysis was also performed to understand the coupling of the self-induced magnetic field and the external magnetic field. Furthermore, the effect of an external magnetic field on the stress distribution in the foil was analysed, based on which the equation of Mode I stress intensity factor for the electromagnetic loading in the presence of an external magnetic field was defined. The results were found to be consistent with the experimental behavior. Finally, the evaluated transient stress intensity factors were compared with the plane stress fracture toughness of a 11μm thick Al foil. A good match was observed between the two, indicating that fracture initiated when (KI transient ≈ KIC). The role of temperature and buckling was also determined while explaining the phenomena using linear elastic fracture mechanics (LEFM).

Keywords: Current density; electromagnetic forces; external magnetic field; stress intensity factor; linear elastic fracture mechanics